

# A note on classical ground state energies

MICHAEL K.-H. KIESSLING

Department of Mathematics, Rutgers University

Piscataway NJ 08854, USA

## Abstract

The pair-specific ground state energy  $\varepsilon_g(N) := \mathcal{E}_g(N)/(N(N-1))$  of Newtonian  $N$  body systems grows monotonically in  $N$ . This furnishes a whole family of simple new tests for minimality of putative ground state energies  $\mathcal{E}_g^x(N)$  obtained through computer experiments. Inspection of several publicly available lists of such computer-experimentally obtained putative ground state energies  $\mathcal{E}_g^x(N)$  has yielded several dozen instances of  $\mathcal{E}_g^x(N)$  which failed one of these tests; i.e., for those  $N$  one concludes that  $\mathcal{E}_g^x(N) > \mathcal{E}_g(N)$  strictly. Although the correct  $\mathcal{E}_g(N)$  is not revealed by this method, it does yield a better upper bound on  $\mathcal{E}_g(N)$  than  $\mathcal{E}_g^x(N)$  whenever  $\mathcal{E}_g^x(N)$  fails a monotonicity test. The surveyed  $N$ -body systems include in particular  $N$  point charges with 2- or 3-dimensional Coulomb pair interactions, placed either on the unit 2-sphere or on a 2-torus (a.k.a. Thomson, Fekete, or Riesz problems).

# 1 Introduction

The pair-specific ground state energy  $\varepsilon_g(N)$  of Newtonian  $N$  body systems exhibits the following monotonic dependence on  $N$ :

**Proposition 1.** *Let  $\Lambda \subset \mathbb{R}^d$  be a bounded and connected domain, and let  $\mathbf{q}_k \in \bar{\Lambda}$ . Assume the following hypotheses on  $U_\Lambda(\check{\mathbf{q}}, \hat{\mathbf{q}})$ :*

- (H1) *Symmetry:*  $U_\Lambda(\check{\mathbf{q}}, \hat{\mathbf{q}}) = U_\Lambda(\hat{\mathbf{q}}, \check{\mathbf{q}})$
- (H2) *Lower Semi-Continuity:*  $U_\Lambda(\check{\mathbf{q}}, \hat{\mathbf{q}})$  is l.s.c. on  $\bar{\Lambda} \times \bar{\Lambda}$ .

For  $N \geq 2$ , define the pair-specific ground state energy by

$$\varepsilon_g(N) \equiv \frac{1}{N(N-1)} \min_{\{\mathbf{q}_1, \dots, \mathbf{q}_N\}} \sum_{1 \leq i < j \leq N} U_\Lambda(\mathbf{q}_i, \mathbf{q}_j). \quad (1)$$

Then the sequence  $N \mapsto \varepsilon_g(N)$  so defined is monotonic increasing.

For the convenience of the reader we here reproduce the elementary proof from Appendix A in [Kie09].

*Proof of Proposition 1:*

We begin by noting that under hypotheses (H1) and (H2) the pair-specific ground state energy  $\varepsilon_g(N)$  defined in (1) is well-defined; i.e.  $\varepsilon_g(N) \in \mathbb{R}$ .

To prove the monotonicity of  $N \mapsto \varepsilon_g(N)$ , with  $N \geq 2$ , let  $\mathcal{E}_g(N)$  denote the  $N$ -body ground state energy, i.e.  $\varepsilon_g(N) = \mathcal{E}_g(N)/(N(N-1))$ . Using the definition of  $\mathcal{E}_g(N)$  and the elementary graph-theoretical identity that the sum over all bonds in a complete  $N$ -graph ( $N > 2$ ) equals  $(N-2)^{-1}$  the sum over all bonds of all its complete  $N-1$ -subgraphs, and using the single inequality that the minimum of a sum is not less than the sum of the minima, we find

$$\begin{aligned} \mathcal{E}_g(N+1) &= \min_{\{\mathbf{q}_1, \dots, \mathbf{q}_{N+1}\}} \sum_{1 \leq i < j \leq N+1} U_\Lambda(\mathbf{q}_i, \mathbf{q}_j) \\ &= \min_{\{\mathbf{q}_1, \dots, \mathbf{q}_{N+1}\}} \frac{1}{N-1} \sum_{1 \leq k \leq N+1} \left[ \sum_{\substack{1 \leq i < j \leq N+1 \\ i \neq k \neq j}} U_\Lambda(\mathbf{q}_i, \mathbf{q}_j) \right] \\ &\geq \frac{1}{N-1} \sum_{1 \leq k \leq N+1} \left[ \min_{\{\mathbf{q}_1, \dots, \mathbf{q}_{N+1}\} \setminus \{\mathbf{q}_k\}} \sum_{\substack{1 \leq i < j \leq N+1 \\ i \neq k \neq j}} U_\Lambda(\mathbf{q}_i, \mathbf{q}_j) \right] \\ &= \frac{N+1}{N-1} \min_{\{\mathbf{q}_1, \dots, \mathbf{q}_N\}} \sum_{1 \leq i < j \leq N} U_\Lambda(\mathbf{q}_i, \mathbf{q}_j) \\ &= \frac{N+1}{N-1} \varepsilon_g(N). \end{aligned} \quad (2)$$

Dividing (2) by  $(N+1)N$  yields  $\varepsilon_g(N+1) \geq \varepsilon_g(N)$ , and the proof of the monotonicity of  $N \mapsto \varepsilon_g(N)$  is complete.  $\square$

As already remarked in Appendix A of [Kie09], Proposition 1 and its proof are quite elementary and presumably known, yet after a serious search in the pertinent literature I came up empty-handed, and additional consultation with several of my local expert colleagues have given me the impression that Proposition 1 is perhaps not known, and in any event not widely known.

In this brief note we will be concerned with a very practical application of Proposition 1 which certainly is not generally known, as we will demonstrate. Namely, the monotonic increase with  $N$  of the true pair-specific ground state energies  $\mathcal{E}_g(N)$  furnishes a whole family of *necessary criteria for minimality* which any empirical list of computer-experimental data  $\{\mathcal{E}_g^x(N); N = 2, 3, 4, \dots, N_*\}$  for such ground state energies needs to satisfy; put differently, we have the following *sufficient criterion for failure to be minimal*:

$$\forall N \geq 2 : (\exists n \geq 1 : \varepsilon_g^x(N+n) < \varepsilon_g^x(N) \implies \mathcal{E}_g^x(N) > \mathcal{E}_g(N)). \quad (3)$$

For each  $n \geq 1$  one can use (3) as a test for any computer-experimentally produced list of putative ground state energies  $\{\mathcal{E}_g^x(N); N = 2, 3, 4, \dots, N_*\}$ . Of course, if any particular  $\mathcal{E}_g^x(N)$  passes the  $n$ -th test for each  $n \leq N_* - N$ , i.e. if  $\varepsilon_g^x(N+n) \geq \varepsilon_g^x(N) \forall n = 1, \dots, N_* - N$ , this does not mean that this  $\mathcal{E}_g^x(N)$  is a true ground state energy; only *failing a test is significant*, for (3) asserts that *a test-failing  $\mathcal{E}_g^x(N)$  is surely not a ground state energy*. Moreover, whenever  $\mathcal{E}_g^x(N)$  fails any such test, then by Proposition 1 we also get a better empirical upper bound on the true ground state energy  $\mathcal{E}_g(N)$  than  $\mathcal{E}_g^x(N)$  from the remaining data of the computer-generated list  $\{\mathcal{E}_g^x(N); N = 2, 3, \dots, N_*\}$ :

$$\mathcal{E}_g(N) \leq \min_{1 \leq n \leq N_* - N} \left\{ \frac{N(N-1)}{(N+n)(N+n-1)} \mathcal{E}_g^x(N+n) \right\}. \quad (4)$$

Note that (4) is always true, but it only leads to a better empirical upper bound on  $\mathcal{E}_g(N)$  than  $\mathcal{E}_g^x(N)$  when  $\mathcal{E}_g^x(N)$  fails a test. Note also that the computer-experimental data supply empirical upper bounds to the actual ground state energies within the numerical accuracy,<sup>1</sup> i.e. we always have  $\mathcal{E}_g^x(N) \geq \mathcal{E}_g(N)$ .

Subjecting some publically available lists of computer-generated data of putative ground state energies  $\mathcal{E}_g^x(N)$  for various  $N$ -body systems to the above tests has yielded several dozen instances of  $\mathcal{E}_g^x(N)$  which failed one of these tests; i.e., for those  $N$  we conclude that  $\mathcal{E}_g^x(N) > \mathcal{E}_g(N)$  strictly, and we get an improved empirical upper bound on  $\mathcal{E}_g(N)$  through (4). The surveyed  $N$ -body systems are  $N$  point charges with  $D$ -dimensional Coulomb pair interactions ( $D = 2; 3$ ), placed either on the unit 2-sphere or on a 2-torus (variably known as (elliptic) Fekete, Thomson, and Riesz problems). The analysis of the sphere data is reported in the next section; for the torus data see section 3.

---

<sup>1</sup>It is assumed here that the algorithms have computed the energy of *some* configuration.

## 2 Many point charges on the 2-sphere

Finding the minimum energy configuration(s) of  $N$  point charges placed on the unit 2 sphere  $\mathbb{S}^2$  is a beautiful, intriguingly rich, and hard mathematical problem which in addition is relevant to many fields of science; see the survey articles [ErHo97], [SaKu97], [AtSu03], and [HaSa04], and the website [Wom09]. One can either interpret  $\mathbb{S}^2$  as a two-dimensional “physical space” in its own right with  $U_{\mathbb{S}^2}(\mathbf{q}_1, \mathbf{q}_2)$  given by the  $D = 2$ -dimensional Coulomb pair interaction  $-\ln|\mathbf{q}_1 - \mathbf{q}_2|$ , where  $|\mathbf{q}_1 - \mathbf{q}_2|$  is the cordal distance on  $\mathbb{S}^2$ ; incidentally, the cordal distance on  $\mathbb{S}^2$  coincides with the three-dimensional Euclidean distance between two points  $\mathbf{q}_1$  and  $\mathbf{q}_2$  on  $\mathbb{S}^2 \subset \mathbb{R}^3$ , but the embedding can be avoided in the discussion. Or, one can interpret  $\mathbb{S}^2 \subset \mathbb{R}^D$  for  $D > 2$  as a proper submanifold, with  $U_{\mathbb{S}^2}(\mathbf{q}_1, \mathbf{q}_2)$  given by the  $D$ -dimensional Coulomb pair interaction  $|\mathbf{q}_1 - \mathbf{q}_2|^{2-D}$ , where  $|\mathbf{q}_1 - \mathbf{q}_2|$  is the  $D$ -dimensional Euclidean distance between two points  $\mathbf{q}_1$  and  $\mathbf{q}_2$  on  $\mathbb{S}^2 \subset \mathbb{R}^D$ . For small  $N$  the ground state configuration (a.k.a. an  $N$ -tuple of Fekete points) can easily be characterized explicitly,<sup>2</sup> and the asymptotic large  $N$ -dependence of  $\mathcal{E}_g(N)$  can be, and to some extent has been [RSZ94] determined analytically without seeking the exact Fekete points,<sup>3</sup> but in general the problem defies analytical treatment. Computer experiments (e.g. [RSZ94], [RSZ95], [Aetal97], [Petal97], [ErHo97], [BCNT02], [BCNT06], [Bet07]) help finding candidates for the minimizing configuration and in any event yield empirical upper bounds  $\mathcal{E}_g^x(N)$  on the ground state energy  $\mathcal{E}_g(N)$ . But even computers are soon overwhelmed because the number of local minimum energy configurations which are not global seems to grow exponentially with  $N$  [ErHo97] so that a computer algorithm is more and more likely to find one of these non-global minima. Indeed, our tests have successfully detected a couple dozen non-global minimum energy values because their pair-specific value surpassed an ensuing empirical pair-specific energy value in some computer-generated list.

### 2.1 Two-dimensional Coulomb interactions

Tables of computer-experimental ground state energies  $\{\mathcal{E}_g^x(N); N = 2, 3, 4, \dots\}$  for  $N$  point charges on  $\mathbb{S}^2$  with two-dimensional Coulomb pair interaction  $U_{\mathbb{S}^2}(\mathbf{q}_1, \mathbf{q}_2) = -\ln|\mathbf{q}_1 - \mathbf{q}_2|$  can be found on the website [BCM], more precisely:

<http://physics.syr.edu/condensedmatter/thomson/shells/...>

[...shelltable.php?topology=sphere&potential=0&start=0&end=5000](http://physics.syr.edu/condensedmatter/thomson/shells/...shelltable.php?topology=sphere&potential=0&start=0&end=5000),

and in [RSZ95], which contains many references to earlier studies.

---

<sup>2</sup>For  $D = 2$  &  $3$  the first dozen minimizers are discussed in the delightful article [AtSu03].

<sup>3</sup>It “suffices” to know that for large  $N$  the Voronoi cells around the charges are mostly hexagons of a certain size; see [SaKu97] for an enlightening discussion. We also remark that the leading order term in the asymptotics can be determined with the help of a very general variational principle, see [KiSp99].

A value of  $\mathcal{E}_g^x(N)$  is listed in [RSZ95] for 199 consecutive values of  $N$  starting at  $N = 2$ ; one also finds there three additional  $\mathcal{E}_g^x(N)$  values for  $N$  which correspond to the icosahedral group. On p.116 of their article, the authors describe various careful tests which they have undertaken to increase the chances of their  $\mathcal{E}_g^x(N)$  actually being  $\mathcal{E}_g(N)$ . In addition to their tests I now have subjected their list of data  $\{\mathcal{E}_g^x(N); N = 2, 3, \dots, 200\}$  to the  $n = 1$  monotonicity test (which, apparently, is not among the tests which the authors of [RSZ95] have used). Their data passed the  $n = 1$  test (there is no point, then, to test with  $n > 1$ ).

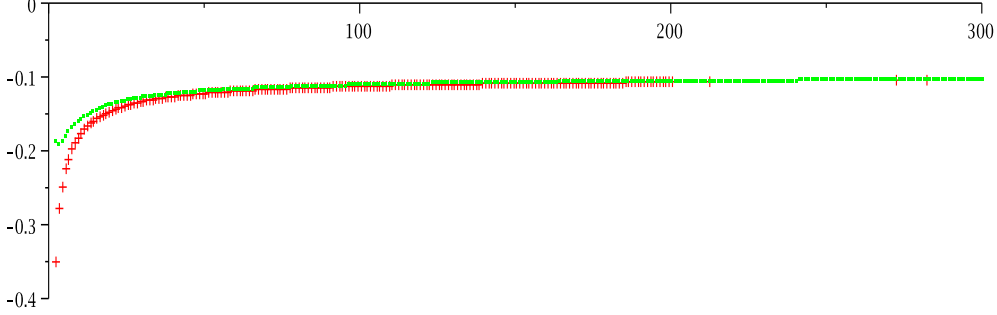
While all tables in [RSZ95] are of course permanent, those at [BCM], according to these authors, are interactive and are updated whenever some user finds a new and better pair  $(N, \mathcal{E}_g^x(N))$ . Therefore it is mandatory to also give the information on which day one downloaded the data from [BCM] for study, which for the computer-experimental data on the  $D = 2$  Coulomb ground state energies I did on Feb. 21, 2009; yet, on Feb. 24, 2009 the crucial data I will be talking about below were still the same. At the time of writing of this paper, this data list  $\{\mathcal{E}_g^x(N); N \in \{3, \dots, 5000\}\}$  has (had) plenty of gaps, i.e. putative ground state energies  $\mathcal{E}_g^x(N)$  are absent for many values of  $N$ . While the absence of the case  $N = 2$  is not a problem, as  $\mathcal{E}_g(2)$  is exactly known, the first real gap is the absence of any  $\mathcal{E}_g^x(11)$ , any  $\mathcal{E}_g^x(19)$ , and soon the gaps become larger and larger. The larger the gaps, the less likely one is to detect non-globally minimizing  $\mathcal{E}_g^x(N)$  with the monotonicity tests, yet two data points “got caught in this net”:  $\mathcal{E}_g^x(97) = -891.653265231 > \mathcal{E}_g(97)$ , for  $\mathcal{E}_g^x(100) - \mathcal{E}_g^x(97) = -0.013678811 < 0$ ; and  $\mathcal{E}_g^x(2000) = -386,187.080630499 > \mathcal{E}_g(2000)$ , for  $\mathcal{E}_g^x(4212) - \mathcal{E}_g^x(2000) = -0.000503199 < 0$ . Notice that while there is only a gap of 2 missing data between  $\mathcal{E}_g^x(97)$  and  $\mathcal{E}_g^x(100)$ , the gap between  $\mathcal{E}_g^x(2000)$  and  $\mathcal{E}_g^x(4212)$  is a whopping 2211. Since the non-globally minimizing  $\mathcal{E}_g^x(2000)$  was detected by the  $n = 2212$  test, it must be quite far away from the actual ground state energy  $\mathcal{E}_g(2000)$ . By (4), and using  $\mathcal{E}_g^x(4212) = -1,722,205.927290610$  from [BCM], we find the upper bound,

$$\mathcal{E}_g(2000) \leq \frac{2000-1999}{4212-4211} \mathcal{E}_g^x(4212) = -388,198.8687. \quad (5)$$

Similarly, with  $\mathcal{E}_g^x(100) = -1,083.376338235$  from [BCM], (4) with  $n=3$  yields  $\mathcal{E}_g(97) \leq \frac{97-96}{100-99} \mathcal{E}_g^x(100) = -1,019.030349$ ; however, this upper bound is certainly beaten by  $\mathcal{E}_g^x(97) = -1,022.023977757$  in [RSZ95]. Incidentally, several other non-globally minimizing data  $\mathcal{E}_g^x(N)$  in the list at [BCM] which actually pass the monotonicity tests can be detected by simply comparing with the list in [RSZ95] (at the time of writing, the non-global data at [BCM] are  $\mathcal{E}_g^x(12)$ ,  $\mathcal{E}_g^x(36)$ ,  $\mathcal{E}_g^x(60)$ ,  $\mathcal{E}_g^x(87)$ ,  $\mathcal{E}_g^x(96)$ ,  $\mathcal{E}_g^x(100)$ ); yet, no such comparison is possible for  $\mathcal{E}_g^x(2000)$  as the data reported in [RSZ95] do not go beyond  $N = 282$ .

We end this subsection with an illustration of the monotonicity of the sequence  $N \mapsto \mathcal{E}_g(N)$  by plotting the monotonically increasing sequence  $N \mapsto$

$\varepsilon_g^x(N) \geq \varepsilon_g(N)$  using the data in [RSZ95], with “=” for  $N \leq 15$  [AtSu03].



Computer-experimental pair-specific ground state energies  $\varepsilon_g^x(N)$  for  $N$  point charges on  $\mathbb{S}^2$  with  $\log r^{-1}$  Coulomb interactions, using the data of [RSZ95] (crosses). Shown also in this plot is the large  $N$  asymptotic two-term approximation to  $\varepsilon_g(N)$  (dots).

Already for  $N > 50$  this empirical curve seems to agree to within less than 1% absolute error with the large  $N$  asymptotics of the actual sequence  $N \mapsto \varepsilon_g(N)$ , given by  $\varepsilon_g(N) \asymp \frac{1}{4} \ln \frac{e}{4} - \frac{1}{4} N^{-1} \ln N + O(N^{-1})$  and obtained through dividing by  $N(N-1)$  the large- $N$  asymptotic formula for  $N \mapsto \mathcal{E}_g(N)$  [RSZ94, RSZ95],

$$\mathcal{E}_g(N) = aN^2 + bN \ln N + O(N) \quad (6)$$

with  $a = \frac{1}{4} \ln \frac{e}{4}$  and  $b = -\frac{1}{4}$ . In [RSZ94] it is also conjectured that, actually,

$$\mathcal{E}_g(N) = aN^2 + bN \ln N + cN + d \ln N + O(1), \quad (7)$$

and rigorous upper and lower bounds on  $c$  are given there. Smale’s 7<sup>th</sup> problem for the 21<sup>st</sup> century asks for an algorithm which upon input  $N$  returns an  $N$ -point configuration on  $\mathbb{S}^2$  for which  $\mathcal{E}_g^x(N)$  does not deviate from  $\mathcal{E}_g(N)$  by more than the fourth term in the conjectured expansion (7) (possibly up to a different coefficient  $d'$ ), and which does so in polynomial time; see [Sma98].

## 2.2 Three-dimensional Coulomb interactions

We next discuss the data for  $N$  point charges on the sphere  $\mathbb{S}^2$  with three-dimensional Coulomb interactions  $U_{\mathbb{S}^2}(\mathbf{q}_1, \mathbf{q}_2) = 1/|\mathbf{q}_1 - \mathbf{q}_2|$ , since [Why52] referred to as “Thomson’s problem” even though Thomson’s “plum pudding model of the atom” [Tho04] is not quite the same problem. Be that as it may, there seem to be many more studies of this Thomson problem than of its variants with other pair interactions and geometries. I perused a sample of those studies and eventually found data which failed a monotonicity test.

Starting at  $N = 2$ , in [ErHo97] one finds 111, and in [RSZ95] 199 consecutively computed putative ground state energies  $\mathcal{E}_g^x(N)$  for the Thomson problem (as just defined). Since the authors in [RSZ95] mention that within

numerical precision their data agree with those on Sloan's home page [HSS94] (actually, at the time: its predecessor via netlib.att.com), I opted for analyzing the data on [HSS94] which are stored (much) more userfriendly than those in [RSZ95] and [ErHo97], even though for only 129 consecutive values of  $N$  some value  $\mathcal{E}_g^x(N)$  is listed, starting with  $N = 4$ , plus a handful of other values for  $N$ s up to  $N = 282$ . All data at [HSS94] passed the  $n = 1$  monotonicity test.

A wonderful treasure of data for the Thomson problem is listed on the website [BCM], more precisely:

<http://physics.syr.edu/condensedmatter/thomson/shells/...>

[...shelltable.php?topology=sphere&potential=1&start=0&end=5000](http://physics.syr.edu/condensedmatter/thomson/shells/...shelltable.php?topology=sphere&potential=1&start=0&end=5000).

I downloaded the data on Feb.09, 2009, and on Feb.24 the relevant data were still present. Starting with  $N = 3$ , one finds computer-experimental ground state energies  $\mathcal{E}_g^x(N)$  for an amazing 1488 consecutive values of  $N$ , the first gap occurring at  $N = 1491$ . In addition one finds almost 300 wider spaced  $\mathcal{E}_g^x(N)$  up to  $N = 5000$ . Quite remarkably, all the consecutive values up to  $N = 1490$  passed the monotonicity test, and so did an additional 70 values of  $\mathcal{E}_g^x(N)$  which are listed with gaps up to  $N = 1800$ . The computer-experimental  $\mathcal{E}_g^x(1801) = 1,579,605.0292504800$  is the first in the list which failed a monotonicity test, in fact the  $n = 1$  test, with  $\varepsilon_g^x(1802) - \varepsilon_g^x(1801) = -0.0000044325$ . Of course, there is also a better upper bound on  $\mathcal{E}_g(1801)$  via (4), but it is not much of an improvement. The story is quite different for the next failing, which is  $\mathcal{E}_g^x(2002) = 2,004,888.5938241700$ , which failed the  $10^{th}$  and the  $20^{th}$  monotonicity tests, with  $\varepsilon_g^x(2012) - \varepsilon_g^x(2002) = -0.0125431412$  and  $\varepsilon_g^x(2022) - \varepsilon_g^x(2002) = -0.012518560$ . This time we obtain two upper bounds from (4) (for  $n = 10$  and  $n = 20$ ), and the better one is for  $n = 10$ , viz.

$$\mathcal{E}_g(2002) \leq \frac{2002 \cdot 2001}{2012 \cdot 2011} \mathcal{E}_g^x(2012) = 1,954,640.745 \quad (8)$$

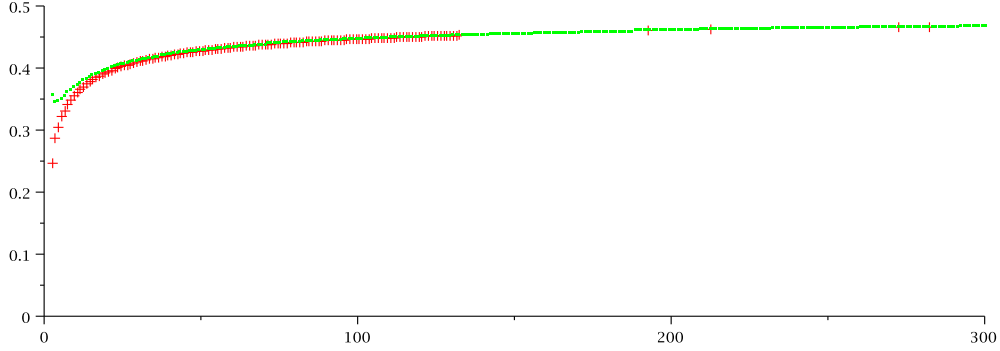
which is also a considerable improvement over the listed  $\mathcal{E}_g^x(2002)$ . Not surprisingly, in this long list of computer-experimental data our harvest is richer than in the previous log list. An additional nine values of  $\mathcal{E}_g^x(N)$  failed one or more of the monotonicity tests (indicated by  $(n = \times)$  behind  $\mathcal{E}_g^x(N)$ ), namely

$$\begin{aligned} \mathcal{E}_g^x(2531) &= 3,204,550.3074368200 \quad (n = 1; 19) \\ \mathcal{E}_g^x(2561) &= 3,207,772.6856023400 \quad (n = 1) \\ \mathcal{E}_g^x(3362) &= 5,543,845.2403717400 \quad (n = 2) \\ \mathcal{E}_g^x(3480) &= 5,941,792.7610333500 \quad (n = 1; 2) \\ \mathcal{E}_g^x(3663) &= 6,586,476.2826423300 \quad (n = 9) \\ \mathcal{E}_g^x(3720) &= 6,793,857.9289983900 \quad (n = 1) \\ \mathcal{E}_g^x(4000) &= 7,860,293.8236758000 \quad (n = 2) \\ \mathcal{E}_g^x(4260) &= 8,920,193.5261720900 \quad (n = 2) \\ \mathcal{E}_g^x(4620) &= 10,498,739.0438109000 \quad (n = 2; 4). \end{aligned}$$

We leave it to the interested reader to use (4) to compute upper bounds on  $\mathcal{E}_g(N)$  for the  $N$  showing in this table and the pertinent  $\mathcal{E}_g^x(N + n)$  at [BCM].

All the data in [Aetal97, Petal97] pass the monotonicity test, but these data are few and far between so that it is actually quite unlikely for any of them to fail a monotonicity test. In fact, [Aetal97] in their table list only five different  $N \in \{2, \dots, 2500\}$  (!), with two different  $\mathcal{E}_g^x(N)$  each; [Petal97] point out that they found a lower energy  $\mathcal{E}_g^x(2472)$  than did [Aetal97]. Also [BCM] provided a putative value for  $N = 2472$ , and their  $\mathcal{E}_g^x(2472) = 2,987,485.953(\dots)$  is even lower than the one in [Petal97], which is  $\mathcal{E}_g^x(2472) = 2,987,486.132$ . Incidentally, there is also a moral here, to be told in the last section.

To illustrate the monotonicity of the sequence  $N \mapsto \varepsilon_g(N)$  I plot the monotonically increasing sequence  $N \mapsto \varepsilon_g^x(N) \geq \varepsilon_g(N)$ , this time using the data in [HSS94]. For  $N \leq 15$  also these two sequences are identical [AtSu03].



Computer-experimental pair-specific ground state energies  $\varepsilon_g^x(N)$  for  $N$  point charges on  $\mathbb{S}^2$  with  $r^{-1}$  Coulomb interactions, using the data of [HSS94] (crosses). Also shown are the leading three terms in the conjectured asymptotic large  $N$  approximation to  $\varepsilon_g(N)$  (dots).

Also shown in this diagram is the *partially conjectured* large  $N$  asymptotics  $\varepsilon_g(N) \asymp \frac{1}{2} - 0.55305(\dots)N^{-1/2} + \frac{1}{2}N^{-1} + O(N^{-3/2})$ , obtained through dividing by  $N(N-1)$  the following large- $N$  asymptotic formula for  $N \mapsto \mathcal{E}_g(N)$ ,

$$\mathcal{E}_g(N) = aN^2 + bN^{3/2} + cN + dN^{1/2} + e + O(N^{-1/2}), \quad (9)$$

where  $a = 1/2$  is the only rigorously proven coefficient [RSZ94], [KuSa98], [KiSp99], while it is conjectured [RSZ94] that  $c = 0 = e$  and

$$b = 3 \left( \frac{\sqrt{3}}{8\pi} \right)^{1/2} \zeta \left( \frac{1}{2} \right) \sum_{k=0}^{\infty} \left( \frac{1}{\sqrt{3k+1}} - \frac{1}{\sqrt{3k+2}} \right) = -0.55305\dots, \quad (10)$$

whereas  $d$  is estimated numerically in [RSZ95].

### 3 Many point charges on a 2-torus

For the perhaps most prominent non-spherical topology, the 2-torus  $\mathbb{T}^2 \subset \mathbb{R}^3$ , we found data lists at [BCM]. However, these lists are clearly preliminary.



### 3.1 Two-dimensional Coulomb interactions

Curiously, at [BCM] putative ground state energies  $\mathcal{E}_g^x(N)$  are only listed for four different values of  $N$ , and all of them are obtained with different aspect ratios of the tori. Hence, no meaningful monotonicity test can be applied.

A visualization of a putative ground state configuration of  $N$  point charges with logarithmic Coulomb interactions on a 2-torus can be found in [HaSa04] and on the cover of that issue of the Notices, and also at [Wom09].

### 3.2 Three-dimensional Coulomb interactions

At [BCM] one finds about 50 data of putative ground state energies  $\mathcal{E}_g^x(N)$  for the aspect ratio 1.414, which are computed for sparsely placed  $N$  up to  $N = 5000$ . For sparsely placed data one would expect it to be less likely to find some which fail a monotonicity test. However, the data  $\mathcal{E}_g^x(N)$  for nine  $N$  failed a monotonicity test for one or more  $n$ , namely:

|                         |   |   |
|-------------------------|---|---|
| $\mathcal{E}_g^x(15)$   | = | 81.390479174 ( $n = 5; 6; 9; 11; 12$ )        |
| $\mathcal{E}_g^x(30)$   | = | 331.088832684 ( $n = 2; 5; 6; 7; 10$ )        |
| $\mathcal{E}_g^x(113)$  | = | 5,370.892624565 ( $n = 4; 7; 38; 49; 78$ )    |
| $\mathcal{E}_g^x(262)$  | = | 28,287.128667479 ( $n = 38; 238; 290$ )       |
| $\mathcal{E}_g^x(360)$  | = | 53,857.158956562 ( $n = 140; 192; 200; 694$ ) |
| $\mathcal{E}_g^x(396)$  | = | 66,660.796433247 ( $n = 104; 156; 164; 598$ ) |
| $\mathcal{E}_g^x(1000)$ | = | 418,396.928796506 ( $n = 363; 4000$ )         |
| $\mathcal{E}_g^x(1363)$ | = | 707,154.008010865 ( $n = 3637$ )              |
| $\mathcal{E}_g^x(3500)$ | = | 5,174,438.587013800 ( $n = 1500$ ).           |

Again, we leave it to the interested reader to use (4) and the above table to compute upper bounds on  $\mathcal{E}_g(N)$  from the pertinent data list at [BCM].

## 4 Some variations on the theme

Two- and three-dimensional Coulomb pair interactions and 2-sphere and 2-torus domains are merely the most prominent examples of pair interactions  $U_\Lambda(\mathbf{q}_i, \mathbf{q}_j)$  and  $d$ -dimensional domains  $\Lambda$  to which Proposition 1 applies. Other, though physically less important, examples of interactions are  $D$ -dimensional Coulomb interactions with  $D > 3$ , and more generally the so-called Riesz interactions, computed with  $U_\Lambda^{(s)}(\mathbf{q}_i, \mathbf{q}_j) = -\text{sign}(s)|\mathbf{q}_i - \mathbf{q}_j|^s$ , for any real  $s < 2$ ; see, e.g. [KuSa98], [HaSa04], [HaSa05], [KSS07], [Bet07]. The logarithmic Coulomb interaction is usually considered to be the special case  $s = 0$ , in the sense that  $\lim_{s \downarrow 0} s^{-1}(|\mathbf{q}_i - \mathbf{q}_j|^{-s} - 1) = -\ln|\mathbf{q}_i - \mathbf{q}_j|$ ; For  $s = 1$  the Riesz energy gives  $U_\Lambda(\mathbf{q}_i, \mathbf{q}_j) = -|\mathbf{q}_i - \mathbf{q}_j|$ , in which case Proposition 1 may shed some new light on the question of the maximum average pair-wise distance of points in  $\Lambda$  and related problems; beside the cited general survey articles, also see

[Bec84]. Proposition 1 applies also to other bounded domains, in particular curves! I should emphasize that the logarithmic interactions between charges constrained to (planar) curves can be studied in quite some detail with complex variable techniques, see [Ketal04]. Proposition 1 can easily be generalized to unbounded domains, with lower semi-continuity replaced by another appropriate condition guaranteeing minimizing configurations for all  $N$ . A physically important example is  $\Lambda = \mathbb{R}^3$  with  $U_{\mathbb{R}^3}(\mathbf{q}_i, \mathbf{q}_j) = |\mathbf{q}_i - \mathbf{q}_j|^{-12} - |\mathbf{q}_i - \mathbf{q}_j|^{-6}$ , which has minimizing  $N$ -body configurations for each  $N$ , known as Lennard-Jones clusters, see [AtSu03] for a recent survey. At the expense of replacing the minimum by an infimum, pair interactions which are merely bounded below can be handled also, but minimizing sequences which don't converge to a minimizing configuration are perhaps less interesting.

## 5 Summary

The main purpose of this article is to draw attention to the monotonicity tests implied by Proposition 1 and to emphasize the ups and downs of this monotonicity test family, not to report on an exhaustive series of such tests covering all available data. In fact, having demonstrated the utility of these tests, it is much more efficient when they are being directly implemented in the computer experiments rather than being run by a third person afterwards.

I still owe the reader the moral announced earlier. Originally I had analyzed the data of computer-experimental ground state energies  $\mathcal{E}_g^x(N)$  reported in [Aetal97] which, divided by  $N(N-1)$ , arranged themselves monotonically increasing when plotted vs.  $N$ ; in fact, this prompted me to conjecture and then prove Proposition 1. But, as we saw, those data are not the correct ground state energies. With hindsight I was quite lucky, for such widely spaced data almost inevitably form a pair-specific monotonic sequence. Had I hit upon a more closely spaced list of non-optimal data which would not have been pair-specifically monotonic, I may not have conjectured the monotonicity in the first place!

**Acknowledgment.** This paper was written with support from the NSF under grant DMS-0807705. Any opinions expressed in this paper are entirely those of the author and not those of the NSF. I like to thank my colleague A. Shadi Tahvildar-Zadeh for going through the painstaking process of verifying that those data which failed a monotonicity test were really there and not made up by me.<sup>4</sup> I also thank József Beck and Doron Zeilberger for their comments on Proposition 1, and Xiaoping Peng for helping me with the data processing.

---

<sup>4</sup>Just in case you take a look and don't find those data anymore which failed a monotonicity test — there were some that did! Incidentally, I myself plan to try to improve on some data which failed a monotonicity test after registering on the interactive website [BCM].

## References

- [Aetal97] Altschuler, E.L., Williams, T.J., Ratner, E.R., Tipton, R., Stong, R., Dowla, F., and Wooten, F.: “Possible global minimum lattice configurations for Thomson’s problem of charges on the sphere,” *Phys. Rev. Lett.* **78**, 2681–2685 (1997).
- [AtSu03] Atiyah, M., and Sutcliffe, P., “Polyhedra in physics, chemistry, and geometry,” *Milan J. Math.* **71**, 33–58 (2003).
- [Bec84] Beck, J., “Sums of distances between points on a sphere — an application of the theory of irregularities of distribution to discrete geometry,” *Mathematica* **31**, 33–41 (1984).
- [Betal07] Bendito, E., Carmona, A., Encinas, A.M., and Gesto, J.M., “Estimation of Fekete points,” *J. Comp. Phys.* **225**, 2354–2376 (2007).
- [BCNT02] Bowick, M.J., Cacciuto, C., Nelson, D.R., and Travesset, A., “Crystalline order on a sphere and the generalized Thomson problem,” *Phys. Rev. Lett.* **89**, 185502ff. (2002).
- [BCNT06] Bowick, M.J., Cacciuto, C., Nelson, D.R., and Travesset, A., “Crystalline particle packings on a sphere with long range power law potentials,” *Phys. Rev.* **B73** 024115ff. (2006).
- [BCM] Bowick, M.J., Cecka, C., and Middleton, A., <http://tristis.phy.syr.edu/thomson/thomson.php>
- [ErHo97] Erber, T., and Hockney, G. M., “Complex systems: equilibrium configurations of  $N$  equal charges on a sphere ( $2 \leq N \leq 112$ ),” pp. 495–594 in *Adv. Chem. Phys.* **XCVIII** (I. Prigogine, S. A. Rice, Eds.), Wiley, New York (1997).
- [HaSa04] Hardin, D.P., and Saff, E.B., “Discretizing manifolds via minimum energy points,” *Notices of the AMS* **51**, 1186–1194 (2004).
- [HaSa05] Hardin, D.P., and Saff, E.B., “Minimal Riesz energy point configurations for rectifiable d-dimensional manifolds,” *Adv. Math.* **193**, 174–204 (2005).
- [HSS94] Hardin, R.H., Sloan, N.J.A., and Smith, W.D., “Minimal energy arrangements of points on a sphere,” ©(1994) HSS; <http://www.research.att.com/~njas/electrons>.
- [KiSp99] Kiessling, M.K.-H., and Spohn, H., “A note on the eigenvalue density of random matrices,” *Commun. Math. Phys.* **199**, 683–695 (1999).
- [Kie09] Kiessling, M.K.-H., “The Vlasov continuum limit for the classical microcanonical ensemble,” *Rev. Math. Phys.* submitted (2009).
- [Ketal04] Kleine Berkenbusch, M., Claus, I., Dunn, C., Kadanoff, L. P., Nicewicz, M., and Venkataramani, S. C., “Discrete charges on a two dimensional conductor,” *J. Stat. Phys.* **116**, 1301–1358 (2004).
- [KuSa98] Kuijlaars, A. B. J., and Saff, E. B., “Asymptotics for minimal discrete energy on the sphere,” *Trans. Amer. Math. Soc.* **350**, 523–538 (1998).
- [KSS07] Kuijlaars, A. B. J., Saff, E. B., and Sun, X., “On separation of minimal Riesz energy points on spheres in Euclidean spaces,” *J. Comput. Appl. Math.* **199**, 172–180 (2007).

- [Petal97] Pérez-Garrido, A., Dodgson, M.J.W., Moore, M.A., Ortuño, M., and Díaz-Sánchez, A., “Comment on: ‘Possible global minimum lattice configurations for Thomson’s problem of charges on a sphere’,” *Phys. Rev. Lett.* **79**, 1417 (1997).
- [RSZ94] Rakhmanov, E.A., Saff, E. B., and Zhou, Y.M., “Minimal discrete energy on the sphere,” *Math. Res. Lett.* **1**, 647–662 (1994).
- [RSZ95] Rakhmanov, E.A., Saff, E. B., and Zhou, Y.M., “Electrons on the sphere,” pp. 111–127 in *Computational Methods and Function Theory* (R. M. Ali, S. Ruscheweyh, and E. B. Saff, eds.), World Scientific, (1995).
- [SaKu97] Saff, E. B., and Kuijlaars, A. B. J., “Distributing many points on a sphere,” *Math. Intelligencer* **19**, 5–11 (1997).
- [Sma98] Smale, S. “Mathematical problems for the next century,” *Math. Intelligencer* **20**, 7–15 (1998); see also version 2 on Steve Smale’s home page: <http://math.berkeley.edu/~smale/>.
- [Tho04] Thomson, J.J., “On the structure of the atom: an investigation of the stability and periods of oscillation of a number of corpuscles arranged at equal intervals around the circumference of a circle; with application of the results to the theory of atomic structure,” *Philos. Mag.* **7**, 237–265 (1904).
- [Why52] Whyte, L.L., “Unique arrangements of points on a sphere,” *Amer. Math. Monthly* **59**, 606–611 (1952).
- [Wom09] Womersley, R.S., Robert Womersley’s home page: <http://web.maths.unsw.edu.au/~rsw/>.